

Modeling the Elastic Mean Free Path of Electron Collision with Pyrimidine: The Screen Corrected Additivity Rule Method

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Abstract : This study presents a comprehensive investigation into the elastic mean free path (EMFP) of electrons colliding with pyrimidine, a precursor to the pyrimidine bases in DNA, employing the Screen Corrected Additivity Rule (SCAR) method. The SCAR method is introduced as a novel approach that combines classical and quantum mechanical principles to elucidate the interaction of electrons with pyrimidine. One of the most fundamental properties characterizing the propagation of a particle in the nuclear medium is its mean free path. Knowledge of the elastic mean free path is essential to accurately predict the effects of radiation on biological matter, as it contributes to the distances between collisions. Additionally, the mean free path plays a role in the interpretation of almost all experiments in which an excited electron moves through a solid. Pyrimidine, the precursor of the pyrimidine bases of DNA, has interesting physicochemical properties, which make it an interesting molecule to study from a fundamental point of view. These include a relatively large dipole polarizability and dipole moment and an electronic charge cloud with a significant spatial extension, which justifies its choice in this present study.

Keywords : elastic mean free path, elastic collision, pyrimidine, SCAR

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